STW-Structure Search 6.18.05

10/644,981

=> d ibib abs hitstr 1-12

L4 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2004:412819 CAPLUS

DOCUMENT NUMBER:

140:423713

TITLE:

Preparation of benzodiazepine derivatives for the

treatment of diabetes mellitus

INVENTOR(S):

Yu, Jinghua; Ghosh, Soumitra S.; Pei, Yazhong

PATENT ASSIGNEE(S):

Mitokor, Inc., USA

SOURCE:

PCT Int. Appl., 64 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT	NO.			KIN	D	DATE		1	APPL	I CAT	ION	NO.		D	ATE	
		-			-									_		
WO 2004	04128	36		A1		2004	0521	1	WO 2	003-1	JS34	340		2	0031	027
W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ĔG,	ES,	FI,	GB,	GD,	GE,
	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	KZ,	LC,	LK,
•	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,
	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	TJ,	TM,
	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW		
RW:	GH,	GM,	ΚE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,
	KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	ΒĒ,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,
	FI,	FR,	GB,	GR,	ΗU,	ΙE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,	TR,
	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG
PRIORITY APPLN. INFO.:							Ī	US 2	002-4	1225	91P		P 2	0021	030	
OTHER SOURCE(S):			MARI	TAS	140:	4237	13									
GI																

The invention provides compns. and methods for altering insulin secretion using a benzodiazepine compound that inhibits calcium efflux via the mitochondrial calcium/ sodium antiporter (MCA). The title compds., e.g. I [R1, R2 = halo; R4 = (un)substituted alkyl, etc.; a provision is given], are prepared Methods of treatment are thereby provided, and are particularly useful for treatment of subjects having, or suspected of being at risk for having, diabetes mellitus. The bioactivities of compds. of this invention were demonstrated.

IT 690999-62-3P 690999-64-5P

Ι

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of benzodiazepine derivs. for the treatment of diabetes mellitus)

RN 690999-62-3 CAPLUS

CN Acetamide, 2-bromo-N-[[2-[(bromoacetyl)amino]-5-chlorophenyl](2chlorophenyl)methyl]-N-[2-(3,4-dimethoxyphenyl)ethyl]- (9CI) (CA INDEX

$$\begin{array}{c|c} & & & \text{OMe} \\ & & &$$

RN 690999-64-5 CAPLUS

CN Acetamide, N-[(2-amino-5-chlorophenyl)(2-chlorophenyl)methyl]-2-bromo-N-[2-(3,4-dimethoxyphenyl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{OMe} \\ \hline & \text{C1} & \text{CH} \\ & \text{CH} & \text{N-CH}_2\text{-CH}_2 \\ \hline & \text{NH}_2 \\ \end{array}$$

ANSWER 2 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2002:669869 CAPLUS 137:352486

DOCUMENT NUMBER: TITLE:

Asymmetric Carbon-Carbon Bond Formations in Conjugate Additions of Lithiated N-Boc Allylic and Benzylic

Amines to Nitroalkenes: Enantioselective Synthesis of Substituted Piperidines, Pyrrolidines, and

Pyrimidinones

AUTHOR (S):

Johnson, Timothy A.; Jang, Doo Ok; Slafer, Brian W.;

Curtis, Michael D.; Beak, Peter

CORPORATE SOURCE:

Department of Chemistry, Roger Adams Laboratory,

SOURCE:

University of Illinois, Urbana, IL, 61801, USA Journal of the American Chemical Society (2002),

124 (39), 11689-11698

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE:

Journal

LANGUAGE: English

(-)-Sparteine mediated lithiations of N-Boc-allylic and benzylic amines AB provide configurationally stable intermediates which on conjugate addns. to nitroalkenes provide highly enantioenriched enecarbamate products in good yields, and with high diastereoselectivities. Straightforward transformations of these adducts offer general routes to substituted 3,4-substituted piperidines, 3,4-substituted pyrrolidines, and 4,5-substituted pyrimidinones. Diastereoselective substitutions of intermediate lactams followed by reduction provide 3,4,5-substituted piperidines and 3,4-trisubstituted pyrrolidines. Lithiation adjacent to nitrogen of 3,4-substituted piperidines and pyrrolidines followed by

CN

diastereoselective substitution opens a route to 2,4,5- and 2,4,5,6-substituted piperidines as well as 2,3,4- and 2,3,4,5-substituted pyrrolidines. The enantiomers of the enecarbamate and 3,4-substituted piperidine products may be accessed by stannylation/transmetalation sequences as well as by further manipulation of 4-substituted piperidones. The methodol. is used to synthesize both enantiomers of an aspartic peptidase inhibitor intermediate, 3-hydroxy-4-phenylpiperidine, as well as the antidepressant (+)-femoxetine.

IT 474924-82-8P 474925-58-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (asym. carbon-carbon bond formations in conjugate addns. of lithiated N-Boc allylic and benzylic amines to nitroalkenes)

RN 474924-82-8 CAPLUS

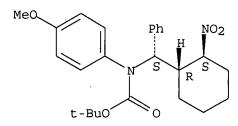
Carbamic acid, (4-methoxyphenyl)[(S)-[(1R,2R)-2-nitrocyclohexyl]phenylmethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 474925-58-1 CAPLUS

CN Carbamic acid, (4-methoxyphenyl)[(S)-[(1R,2S)-2-nitrocyclohexyl]phenylmethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 3 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:658081 CAPLUS

47

DOCUMENT NUMBER: 137:185493

TITLE: Preparation of 1,3-diaminopropanes as analgesics INVENTOR(S): Sundermann, Bernd; Buschmann, Helmut: Koegel.

Sundermann, Bernd; Buschmann, Helmut; Koegel,
Babette-Yvonne; Merla, Beatrix; Risch, Nikolaus

PATENT ASSIGNEE(S): Gruenenthal G.m.b.H., Germany

SOURCE: PCT Int. Appl., 92 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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KIND
                                DATE
                                            APPLICATION NO.
                                                                   DATE
     PATENT NO.
                         ____
                                            ______
     WO 2002066432
                                20020829
                                            WO 2002-EP1765
                                                                   20020220
                         A1
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM,
             HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS,
             LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL,
             PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,
             UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ,
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                                20020829
                                            DE 2001-10108307
     DE 10108307
                          A1
                                                                   20010221
     CA 2438704
                          AΑ
                                20020829
                                            CA 2002-2438704
                                                                    20020220
     EP 1363885
                                            EP 2002-714169
                          A1
                                20031126
                                                                   20020220
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     BR 2002007535
                                            BR 2002-7535
                          Α
                                20040309
                                                                    20020220
     JP 2005503330
                          T2
                                20050203
                                            JP 2002-565949
                                                                   20020220
     NO 2003003697
                          Α
                                20031017
                                            NO 2003-3697
                                                                   20030820
     US 2004067928
                          A1
                                20040408
                                            US 2003-644981
                                                                   20030821
                          Α
     ZA 2003007321
                                20050110
                                            ZA 2003-7321
                                                                   20030918
PRIORITY APPLN. INFO.:
                                            DE 2001-10108307
                                                                A 20010221
                                            WO 2002-EP1765
                                                                W 20020220
AB
     R2(NR3R4)CHR1CHCH(NR5R6)A [I; R1 = alkyl, cycloalkyl, alkylcycloalkyl,
     aryl; R2 - alkyl, cycloalkyl, aryl, alkylcycloalkyl, alkylaryl,
     heterocyclyl, alkylheterocyclyl; whereby R1 and R2 can not be together
     aryl and heterocyclyl, or R1R2 = (substituted) (benzocondensed) (CH2)m; m
     = 2-6; R3 = H, alkyl, cycloalkyl, alkylcycloalkyl, alkylaryl,
     heterocyclyl, alkylheterocyclyl, COR7; or R3R4 = (substituted) (CH2)n,
     (CH2)2X(CH2)2; n = 3-7; X = O, S, NR8; R5, R6 = alkyl, cycloalkyl, aryl,
     alkylcycloalkyl, alkylaryl; or R5R6 = (substituted) (CH2)o, (CH2)2Y(CH2)2;
     Y = 0, S, NR9; O = 3-7; A = aryl, heteroaryl, CO2R10, 2-propyl; R7 =
     alkyl, cycloalkyl, aryl, heterocyclyl, alkylcycloalkyl, alkylaryl,
     alkylheterocyclyl; R8, R9 = H, alkyl, cycloalkyl, aryl, alkylcycloalkyl,
     alkylaryl, heterocyclyl; R10 = alkyl, cycloalkyl, aryl, alkylcycloalkyl,
     alkylaryl], were prepared as racemate or in the form of diastereomers or
     enantiomers. Tested I at 10 mg/kg i.v. in mice gave 34-85%
     phenylquinone-induced Writhing.
IT
     187463-24-7P 452093-15-1P 452093-27-5P
     452093-30-0P 452093-35-5P 452093-38-8P
     452093-42-4P 452093-45-7P 452093-47-9P
     452093-51-5P 452093-55-9P 452093-58-2P
     452093-64-0P 452093-70-8P 452093-75-3P
     452093-80-0P 452093-84-4P 452093-90-2P
     452093-94-6P 452093-97-9P 452093-99-1P
     452094-01-8P 452094-03-0P 452094-05-2P
     452094-07-4P 452094-09-6P 452094-12-1P
     452094-16-5P 452094-19-8P 452094-23-4P
     452094-28-9P 452094-34-7P 452094-37-0P
     452094-40-5P 452094-46-1P 452094-52-9P
     452094-58-5P 452094-61-0P 452094-64-3P
     452094-67-6P 452094-70-1P 452094-73-4P
     452094-76-7P 452094-79-0P 452094-86-9P
     452094-91-6P 452094-94-9P 452094-97-2P
     452095-00-0P 452095-03-3P 452095-06-6P
     452095-09-9P 452095-12-4P 452095-15-7P
    452095-20-4P 452095-24-8P 452095-28-2P
     452095-31-7P 452095-33-9P 452095-35-1P
     452095-37-3P 452095-39-5P 452095-41-9P
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452095-43-1P 452095-45-3P 452095-48-6P

RN 452095-70-4 CAPLUS

CN Acetamide, N-[(1R,2R)-2-[(R)-(dimethylamino)(2-methoxyphenyl)methyl]cyclohexyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 452095-71-5 CAPLUS

CN Acetamide, N-[(1R,2R)-2-[(R)-(dimethylamino)(2-nitrophenyl)methyl]cyclohexyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 452095-74-8 CAPLUS

CN Benzenemethanamine, N,N-dimethyl- α -[(1R,2S)-2-(propylamino)cyclohexyl]-, (α R)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

L4 ANSWE

ACCESSION NUMBER:

2002:619639 CAPLUS

DOCUMENT NUMBER:

138:89325

TITLE:

Efficient synthesis of diastereomerically pure

1,3-diamines

AUTHOR (S):

Merla, Beatrix; Risch, Nikolaus

CORPORATE SOURCE:

Fachbereich Chemie und Chemietechnik, Universitat

Paderborn, Paderborn, 33098, Germany

SOURCE:

Synthesis (2002), (10), 1365-1372 CODEN: SYNTBF; ISSN: 0039-7881

PUBLISHER:

Georg Thieme Verlag

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 138:89325

AB The reinexpe

The regio- and diastereoselective synthesis of 1,3-diamines using inexpensive starting materials is described. β -Aminoketones are

easily transformed diastereoselectively into syn, anti-, anti-, or anti, syn-1,3-diamines using different methodologies. The configuration

of the products was determined by NMR.

IT 187463-24-7P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(deprotection of; preparation of regio- and diastereomerically pure diamines from generating aminolytopage and their configuration)

from corresponding aminoketones and their configuration)

RN 187463-24-7 CAPLUS

CN Benzenemethanamine, N,N-dimethyl- α -[(1R,2S)-2-

[(phenylmethyl)amino]cyclohexyl]-, (\alpha R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 452093-15-1P 452093-27-5P 452093-30-0P

452093-35-5P 452093-38-8P 452093-42-4P

452093-45-7P 452093-47-9P 452093-51-5P

452093-55-9P 452093-58-2P 452093-64-0P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation of regio- and diastereomerically pure diamines from

corresponding aminoketones and their configuration)

RN 452093-15-1 CAPLUS

CN Benzenemethanamine, α -[(1R,2S)-2-aminocyclohexyl]-N,N-dimethyl-,

 (αR) -rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 452093-27-5 CAPLUS

CN Benzenemethanamine, $\alpha - \{(1R, 2S) - 2 - \text{aminocyclohexyl}\} - 2 - \text{chloro-N.N-}$

(reduction of; preparation of regio- and diastereomerically pure diamines

from

corresponding aminoketones and their configuration)

RN 485403-30-3 CAPLUS

Benzenemethanamine, $\alpha - \{(1R, 2R) - 2 - azidocyclohexyl\} - N, N-dimethyl-,$ CN (αS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

485403-31-4 CAPLUS RN

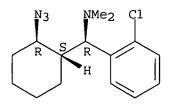
Benzenemethanamine, α -[(1R,2R)-2-azidocyclohexyl]-2-chloro-N,N-CNdimethyl-, (aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 485403-32-5 CAPLUS

Benzenemethanamine, α -[(1R,2S)-2-azidocyclohexyl]-2-chloro-N,N-CN dimethyl-, (αS) -rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT:

THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS 31 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

CAPLUS COPYRIGHT 2005 ACS on STN ANSWER 5 OF 12

ACCESSION NUMBER:

2000:634954 CAPLUS

DOCUMENT NUMBER:

133:218841

TITLE:

Mixed herbicide compositions

INVENTOR(S):

Kobayashi, Kazunori; Ono, Yoshimasa; Miyazawa,

Takeshige

PATENT ASSIGNEE(S):

Kumiai Chemical Industry Co., Ltd., Japan

SOURCE:

Jpn. Kokai Tokkyo Koho, 6 pp. CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

GI

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000247814	A2	20000912	JP 1999-53557	19990302
PRIORITY APPLN. INFO.:			JP 1999-53557	19990302
OTHER SOURCE(S):	MARPAT	133:218841		

$$\begin{array}{c|c} X & NH-SO_2-CHF_2 \\ \hline & N & OMe \\ \hline & V & N \end{array}$$

Mixed herbicides active for a long period, controlling weeds such as barnyard grass, after a single application to flooded rice paddies, are presented. Sulfonyl anilide derivative of I, where X = alkoxyalkyl; Y = alkylamino, in combination with the following compds., namely, 2-chloro-2',6'-diethyl-N-(n-propoxyethyl)-acetanilide, N-butoxymethyl-2-chloro-2',6'-dimethylacetanilide, 2-[4-(2',4'-dichloro-m-toluoyl)-1,3-dimethylpyrazole-5-yloxy]-4-Me acetophenone, 2-(2,4-dichloro-3-methylphenoxy)propionic anilide, 2-bromo-N-(α,α-dimethylbenzyl)-3,3-dimethyl-butylamide or 3-(4-chloro-5-cyclopentyl-oxy-2-fluorophenyl)-5-isopropylidene-1,3-oxazolidine-2,4-dione are claimed.
IT 291291-31-1 291291-32-2 291291-33-3

IT 291291-31-1 291291-32-2 291291-33-3 291291-34-4 291291-35-5 291291-36-6 291291-38-8 291291-42-4 291291-47-9 291291-48-0

RL: AGR (Agricultural use); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process); USES (Uses) (mixed sulfonylanilide herbicide compns.)

RN 291291-31-1 CAPLUS

CN Acetamide, 2-chloro-N-(2,6-diethylphenyl)-N-(2-propoxyethyl)-, mixt. with N-[2-[(diethylamino)(4,6-dimethoxy-2-pyrimidinyl)methyl]-6- (methoxymethyl)phenyl]-1,1-difluoromethanesulfonamide (9CI) (CA INDEX NAME)

CM 1

CRN 221204-49-5 CMF C20 H28 F2 N4 O5 S

MeO N NMe2 CH2-OMe
$$F_2$$
CH-S-NH O

CM 2

CRN 84496-56-0 CMF C16 H15 C12 N O2

RN 291291-48-0 CAPLUS

CN Butanamide, 2-bromo-3,3-dimethyl-N-(1-methyl-1-phenylethyl)-, mixt. with N-[2-[(4,6-dimethoxy-2-pyrimidinyl)(dimethylamino)methyl]-6- (methoxymethyl)phenyl]-1,1-difluoromethanesulfonamide (9CI) (CA INDEX NAME)

CM 1

CRN 221204-54-2 CMF C18 H24 F2 N4 O5 S

MeO NMe2 CH2-OMe
$$F_2CH-S-NH$$
O

CM 2

CRN 74712-19-9

CMF C15 H22 Br N O

L4 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1999:147774 CAPLUS

DOCUMENT NUMBER:

130:223289

TITLE:

Preparation of sulfonanilide moiety containing

pyrimidine derivatives as herbicides

INVENTOR (S):

Yoshimura, Isao; Miyazaki, Masahiro; Suzuki, Senji; Nakaya, Masao; Tamaru, Masatoshi; Ono, Yoshimasa; Ida,

Tomohisa; Yanagisawa, Katsutada; Sadohara, Hideo

PATENT ASSIGNEE(S):

Kumiai Chemical Industry Co., Ltd., Japan; Ihara

Chemical Industry Co., Ltd.

SOURCE:

Jpn. Kokai Tokkyo Koho, 57 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

PE: Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11060562	A2	19990302	JP 1998-173980	19980605
PRIORITY APPLN. INFO.:			JP 1997-169454 A	19970611
OTHER SOURCE(S):	MARPAT	130:223289		

GΙ

AB The title compds. I [R1 = (un)substituted alkyl, etc.; R2 = H, halo, etc.; R3 = H, alkyl, etc.; Q = CH(NR4R5), etc.; m = 1 -4; R4, R5 = H, alkyl, etc.] are prepared The title compound II (at 100 g/10 are) gave \geq 90% control of Scirpus juncoides.

IT 221203-43-6P 221203-44-7P 221203-45-8P 221203-48-1P 221203-49-2P 221203-50-5P 221203-51-6P 221203-52-7P 221203-53-8P 221203-54-9P 221203-55-0P 221203-56-1P 221203-57-2P 221203-58-3P 221203-59-4P 221203-60-7P 221203-61-8P 221203-91-4P 221203-95-8P 221203-96-9P 221203-97-0P 221203-98-1P 221203-99-2P 221204-00-8P 221204-01-9P 221204-02-0P 221204-27-9P

RN 221205-66-9 CAPLUS

CN Methanesulfonamide, N-[2-[(4,6-dimethoxy-2-pyrimidinyl)(methyl-2-propynylamino)methyl]-6-(methoxymethyl)phenyl]-1,1-difluoro-(9CI) (CA INDEX NAME)

Me OMe N-CH₂-C=CH

N CH CH₂-OMe

$$F_2$$
CH-S-NH

L4 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1998:355784 CAPLUS

DOCUMENT NUMBER:

129:136152

TITLE:

N-phenyl-1-aza-2-cyano-1,3-butadienes: an

intramolecular hetero Diels-Alder strategy for the

construction of 1,4-benzodiazepines

AUTHOR(S):

Goulaouic-Dubois, Catherine; Adams, David R.; Sisti,

Nicholas J.; Fowler, Frank W.; Grierson, David S.

CORPORATE SOURCE:

Inst. Chimie Substances Naturelles, CNRS,

Gif-sur-Yvette, 91198, Fr.

SOURCE:

Tetrahedron Letters (1998), 39(24), 4283-4286

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER:

Elsevier Science Ltd.

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 129:136152

AB A new approach to the construction of tricyclic 1,4-benzodiazepines was developed, based upon the intramol. Diels-Alder reaction of 2-cyano-1-azadienes [i.e., [2-[2-[(2-propenylamino)methyl]phenyl]imino]-3-butenenitriles]. This study revealed the difficulties inherent to the direct transformation of an imine-amide to an azadiene, but demonstrated

the efficiency of the intramol. [4+2] cycloaddn. of azadienes as a means to access benzodiazepines. The target compound was 3,4,4a,5-tetrahydro-7phenylpyrido[1,2-a][1,4]benzodiazepine-1-carbonitrile.

IT 210534-47-7P 210534-48-8P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of phenylpyridobenzodiazepinecarbonitrile via Diels-Alder reaction of [[(propenylamino)methyl]phenylimino]butenenitrile)

RN 210534-47-7 CAPLUS

2-Propenamide, N-[2-[phenyl[2-propenyl(trifluoroacetyl)amino]methyl]phenyl CN]- (9CI) (CA INDEX NAME)

RN 210534-48-8 CAPLUS

Acetamide, N-[[2-[(1-cyano-2-propenyl)amino]phenyl]phenylmethyl]-2,2,2-CN trifluoro-N-2-propenyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 8 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1997:129715 CAPLUS

DOCUMENT NUMBER:

126:186041

TITLE:

A simple and highly diastereoselective one-pot

AUTHOR (S):

synthesis of 1,3-diamines

CORPORATE SOURCE:

Merla, Beatrix; Arend, Michael; Risch, Nikolaus Fachbereich Chemie Chemietechnik, Universitaet-Gesamthochschule Paderborn, Paderborn, D-33098,

Germany

SOURCE:

Synlett (1997), (2), 177-178 CODEN: SYNLES; ISSN: 0936-5214

PUBLISHER:

Thieme Journal

DOCUMENT TYPE: LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 126:186041

GI

A convenient 1-pot procedure for the highly diastereoselective synthesis AB of 1,3-diamines from inexpensive starting materials is described. Enamines (E)-R2CH: CR3NR12 [R12 = (CH2)4, R2R3 = (CH2)4 or R2 = Me, R3 = Ph; R12 = (CH2)2O(CH2)2, R2R3 = (CH2)4 or R2 = Me, R3 = Ph, Et; R1 = Et, R2 = Me, R3 = Ph] are aminoalkylated with preformed [PhCH:N+R2]Cl- [R = Me; R2 = (CH2)4, (CH2)2O(CH2)2, (CH2)5] yielding exclusively the corresponding quaternary iminium salts I. In-situ reduction of the latter with NaBH4/MeOH provides a broad access to the corresponding 1,3-diamines II in 42-85% yield.

ΙT 187463-24-7P

> RL: SPN (Synthetic preparation); PREP (Preparation) (stereoselective synthesis of diamines)

RN 187463-24-7 CAPLUS

Benzenemethanamine, N,N-dimethyl- α -[(1R,2S)-2-CN[(phenylmethyl)amino]cyclohexyl]-, (\alpha R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 9 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:531525 CAPLUS

DOCUMENT NUMBER: 117:131525

TITLE: Cycloaddition reactions of γ -amino

> α, β -didehydro amino acid esters: a test case for the principle of 1,3-allylic strain Reetz, Manfred T.; Kayser, Frank; Harms, Klaus

AUTHOR (S):

CORPORATE SOURCE: Max-Planck-Inst. Kohlenforsch., Muelheim/Ruhr, 4330,

Germany

SOURCE: Tetrahedron Letters (1992), 33(24), 3453-6

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal LANGUAGE: English

143250-68-4P

OTHER SOURCE(S): CASREACT 117:131525

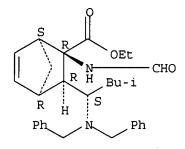
N, N-dibenzylamino aldehydes (PhCH2) 2NCHRCHO (R = Me, PhCH2, Me2CH, Me2CHCH2, Me3CSiMe2OCH2), readily accessible from amino acids, can be converted into γ -N,N-dibenzylamino α , β -didehydro amino acid esters (Z) - and (E) - (PhCH2) 2NCHRCH: C(NHCHO) CO2Et (I) without racemization. (2)-I undergo stereoselective Diels-Alder reactions and 1,3-dipolar cycloaddn. with diazomethane, the sense of diastereoselectivity being opposite to that predicted by the conventional principle of 1,3-allylic strain. IT

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 143250-68-4 CAPLUS

CN Bicyclo[2.2.1]hept-5-ene-2-carboxylic acid, 3-[1-[bis(phenylmethyl)amino]-3-methylbutyl]-2-(formylamino)-, ethyl ester, [1S-[1α , 2β , 3β (R*), 4α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1992:214485 CAPLUS

DOCUMENT NUMBER:

116:214485

TITLE:

SOURCE:

Preparation of 4-benzylisoxazoles as herbicides Cain, Paul A.; Cramp, Susan Mary; Little, Gillian M.

INVENTOR(S):

Rhone-Poulenc Agriculture Ltd., UK

PATENT ASSIGNEE(S):

Eur. Pat. Appl., 31 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE		
	A1	19920212	EP 1991-307351	-	19910809		
EP 470856	B1	19951011					
R: AT, BE, CH,	DE, DK	, ES, FR,	GB, GR, IT, LI, LU, NI	ı, S	Ε		
AU 9181678	A1	19920213	AU 1991-81678		19910807		
AU 643310	B2	19931111					
CA 2048705	AA	19920211	CA 1991-2048705		19910808		
RO 109941	B1	19950728	RO 1991-148219		19910808		
IL 99132	A1	19951231	IL 1991-99132		19910808		
FI 9103782	A	19920211	FI 1991-3782		19910809		
HU 58188		19920228	HU 1991-2664		19910809		
BR 9103433	A	19920519	BR 1991-3433		19910809		
ZA 9106305	A	19921028	ZA 1991-6305		19910809		
JP 05345770	A2	19931227	JP 1991-200537		19910809		
AT 128972	E	19951015	AT 1991-307351		19910809		
ES 2077806	Т3	19951201	ES 1991-307351		19910809		
RU 2055072	C1	19960227	RU 1991-5001315		19910809		
CZ 282110	B6	19970514	CZ 1991-2473		19910809		
CN 1058777	Α	19920219	CN 1991-105623		19910810		
US 5656573	Α	19970812	US 1995-460093		19950602		
PRIORITY APPLN. INFO.:			GB 1990-17539	Α	19900810		
			GB 1989-20519	Α	19890911		
			US 1990-580795	B2	19900911		
•			GB 1990-25469	Α	19901122		
			GB 1991-16833	Α	19910805		
			GB 1991-16835	Α	19910805		

US	1991-742381	B2	19910808
US	1991-790175	B2	19911112
US	1992-850031	B2	19920312
US	1992-850035	B2	19920312
US	1992-850128	B2	19920312
US	1992-850424	B2	19920312
TIC	1993-108792	R1	19930819

OTHER SOURCE(S):

MARPAT 116:214485

GI

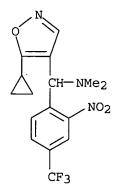
AB Title compds.I; R1 = (halo)alkyl, (halo)alkenyl, (halo)alkynyl, (substituted) cycloalkyl, cycloalkenyl, alkoxycarbonyl, aryl, aralkyl, amino, halo, CHO, etc.; R2 = NO2, cyano, halo, (halo)alkyl, alkylthio, alkylsulfinyl, alkylsulfonyl, sulfamoyl, alkoxycarbonyl, CHO, (thio)carbamoyl, alkoxy, alkoxyalkyl, etc.; R6 = H, OH, halo, (halo)alkyl, (halo)alkenyl, (substituted) cycloalkyl alkylthio, alkylsulfinyl, alkylsulfonyl, cyano, CHO, (thio)carbamoyl, alkoxy, PhO, PhCH2O, PhCO2, (acyl)amino, heterocyclyl, etc.; R7 = H (haloalkyl; R6R7 = (cyclic) (thio)ketal moiety; n = 1-5], were prepared Thus, 4-(2-nitro-4-trifluoromethylbenzoyl)-5-cyclopropylisoxazole (preparation given) was reduced with NaBH4 in EtOH to give title compound II. Numerous I at 1000 g/ha gave ≥90% reduction in growth of ≥1 weed.

IT 141111-96-8P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as herbicide)

RN 141111-96-8 CAPLUS

4-Isoxazolemethanamine, 5-cyclopropyl-N,N-dimethyl- α -[2-nitro-4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



CN

L4 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1990:157881 CAPLUS

DOCUMENT NUMBER:

112:157881

TITLE:

2-Hydroxy-3-aryloxypropylamine derivatives having

cardiovascular activity

Casagrande, Cesare; Santangelo, Francesco; Calabi, INVENTOR(S):

Maria Luisa

PATENT ASSIGNEE(S): Societa Italiana Medicinali e Sintetici S.p.A.

(SIMES), Italy

SOURCE: Eur. Pat. Appl., 19 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 333938	A1 '	19890927	EP 1988-202681	19881124
EP 333938	B1	19930414		
R: AT, BE, CH,	DE, ES	, FR, GB, GR	, IT, LI, LU, NL, SE	
AT 88176	E	19930415	AT 1988-202681	19881124
ES 2054790	Т3	19940816	ES 1988-202681	19881124
US 5047425	Α	19910910	US 1988-278205	19881130
JP 02000241	A2	19900105	JP 1988-305093	19881201
PRIORITY APPLN. INFO.:			IT 1987-22824 A	19871201
			EP 1988-202681 A	19881124

OTHER SOURCE(S): MARPAT 112:157881

ArOCH2CH(OH)CH2NHCRR1XNR2(CH2)nCHR3R4 [I; Ar = (un)substituted cyclic or bicyclic (hetero)aromatic group; R, R1 = H, C1-3 alkyl; X = (CH2)pY; Y = CH2, CO; p = 0, 1, 2; R2 = H, C1-3 alkyl; n = 0, 1, 2; R3, R4 = (un) substituted Ph] having β-blocking activity, thus useful as cardiovascular agents, e.g. in treatment of hypertension, angina pectoris, and heart arrhythmia, are prepared by (1) reaction of H2NCRR1XNR2(CH2)nCHR3R4 with aryl glycidyl ether or ClCH2CH(OH)CH2OAr or (2) alkylation of ArOCH2CH(OH)CH2NHCRR1XNHR2 with N(CH2)nCHR3R4 (W = Cl, Br, MeSO3, p-Me(OH4SO3). Thus, a solution of H2NCMe2CH2NMeCH2CHPh2 and 1,2-epoxy-3-(2-methoxyphenoxy) propane in PhMe was refluxed 4 h to give, after silica gel chromatog. and acidification with HCl in EtOAc, 2-MeOC6H4OCH2CH(OH)CH2NHCMe2CH2NMeCH2CHPh2.2HCl. 2-MeOC6H4OCH2CH(OH)CH2NHCH2CHMeCH2NMeCHPh2 had a high affinity towards the β 1 and β 2 receptors in quinea pig atria comparable to that of a known β -blocker, Propranolol.

ΙT 126059-35-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as β -blocker)

RN126059-35-6 CAPLUS

CN 2-Propanol, 1-[[1,1-dimethyl-2-[methyl[(2-nitrophenyl)phenylmethyl]amino]e thyl]amino]-3-(2-methoxyphenoxy)- (9CI) (CA INDEX NAME)

ANSWER 12 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1978:49955 CAPLUS

DOCUMENT NUMBER:

88:49955

TITLE:

Photochemical studies on an aromatic

amine-polychloromethane system. Part V. Mechanism of

photochemical reactions in the system N.N-dimethylaniline-methylene chloride

AUTHOR (S):

Latowski, Tadeusz; Zelent, Bogumil

CORPORATE SOURCE:

SOURCE:

Inst. Chem., Univ. Gdansk, Gdansk, Pol.
Roczniki Chemii (1977), 51(7-8), 1405-20

CODEN: ROCHAC; ISSN: 0035-7677

DOCUMENT TYPE:

LANGUAGE:

Journal English

GΙ

$$CH_2$$
 N^+Me_2 Cl^-

AB The mechanism of the photochem. reaction of PhNMe2 with aqueous CH2Cl2 involves the formation of PhNMe2+• and •CH2Cl (via an exciplex) which combine to form I which is autoxidized to give p-Me2NC6H4CHO. This mechanism was confirmed by the photoreaction of CH2Cl2 with PhNEt2, Me(p-Me2NC6H4CH2)NPh, or (p-Me2NC6H4)2CH2.

IT 65295-95-6P

RN 65295-95-6 CAPLUS

CN Methanediamine, 1-(2-aminophenyl)-1-(4-aminophenyl)-N,N,N',N'-tetraethyl-(9CI) (CA INDEX NAME)

=> d his

(FILE 'HOME' ENTERED AT 17:46:12 ON 16 JUN 2005)

FILE 'REGISTRY' ENTERED AT 17:46:24 ON 16 JUN 2005

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 178 S L1 FULL

FILE 'CAPLUS' ENTERED AT 17:47:08 ON 16 JUN 2005

L4 12 S L3

=> d 11

L1 HAS NO ANSWERS

L1 STR

0 | | 1_0_g1

- G1 Cb,Ak
- G2 Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,Cy,[@1]

Structure attributes must be viewed using STN Express query preparation.

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